

Griffiths-McCoy singularities in random quantum spin chains: Exact results through renormalization

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The Ma-Dasgupta-Hu renormalization group (RG) scheme is used to study singular quantities in the Griffiths phase of random quantum spin chains. For the random transverse-field Ising spin chain we have extended Fisher's analytical solution to the off-critical region and calculated the dynamical exponent exactly. Concerning other random chains we argue by scaling considerations that the RG method generally becomes asymptotically exact for large times, both at the critical point and in the whole Griffiths phase. This statement is checked via numerical calculations on the random Heisenberg and quantum Potts models by the density matrix renormalization group method.

In a random quantum system at zero temperature several physical quantities are singular not only at the critical point, but in a whole region, as well, which extends on both sides of the transition point [1]. In this Griffiths phase [2] a random quantum system is non-critical in the space direction (spatial correlations decay exponentially), whereas it is critical in the time direction and the corresponding behavior due to Griffiths-McCoy singularities [2,3] is controlled by a line of semi-critical fixed points characterized by the dynamical exponent $z(\delta)$, which depends on the value of the quantum control-parameter, δ . For example average autocorrelations decay in (imaginary) time, τ , as $\sim \tau^{-z(\delta)}$; for a small magnetic field, $H \rightarrow 0$, the magnetization behaves as $\sim H^{1/z(\delta)}$; the low temperature susceptibility and specific heat are singular as $\sim T^{1/z(\delta)-1}$ and $\sim T^{1/z(\delta)}$, respectively. Let us mention that Griffiths-McCoy singularities are relevant in experiments on quantum spin glasses [4] and provides a theoretical explanation about the non-Fermi liquid behavior in U and Ce intermetallics [5].

Among the theoretical methods developed to study random quantum systems the renormalization group (RG) scheme introduced by Ma, Dasgupta and Hu [6] plays a special rôle. For a class of systems, the critical behavior of those is controlled by an infinite-randomness fixed point [7] (IRFP), the RG method becomes asymptotically exact during iteration. For some one-dimensional models, random transverse-field Ising model [8] (RTIM) and the random XXZ-model [9], Fisher has obtained analytical solution of the RG equations and in this way many new exact results and new physical insight about the critical behavior of these models have been gained. Subsequent analytical [10] and numerical [11,10] investigations of the models are in agreement with Fisher's results. The RG-scheme has been numerically implemented in higher dimensions [7,12], as well, to study the critical behavior of the RTIM and rea-

sonable agreement with the results of quantum Monte-Carlo simulations [13] has been found. Considering the Griffiths-phase of random quantum spin chains here the RG-scheme has been rarely used [12], mainly due to the general belief that the method loses its asymptotically exact properties by leaving the vicinity of the scale invariant critical point.

Our aim in the present Letter is to clarify the applicability of the Ma-Dasgupta-Hu RG-method in the Griffiths phase of random quantum spin chains. We start with the RTIM, extend Fisher's calculation [8] to the Griffiths phase of the model and present the analytical solution of the RG-equations. Then, for general models, we analyze by scaling considerations the structure of the RG equations around the line of semi-critical fixed points and arrive to the conclusion that the RG method becomes asymptotically exact in the whole Griffiths region. This statement is then checked numerically on the random Heisenberg chain and the random quantum Potts model (RQPM) using the density matrix renormalization group (DMRG) method.

We start with the 1d RTIM which is defined by the Hamiltonian:

$$H_I = - \sum_i J_i \sigma_i^x \sigma_{i+1}^x - \sum_i h_i \sigma_i^z, \quad (1)$$

where the $\sigma_i^{x,z}$ are Pauli matrices at site i and J_i and h_i are the couplings and the transverse fields, respectively, which are independent random variables. The quantum control-parameter of the model is defined as

$$\delta = \frac{[\ln h]_{\text{av}} - [\ln J]_{\text{av}}}{\text{var}[\ln h] + \text{var}[\ln J]}, \quad (2)$$

where $\text{var}[x]$ is the variance of x and we use $[\dots]_{\text{av}}$ to denote averaging over quenched disorder. For $\delta > 0$ ($\delta < 0$) the system is in the paramagnetic (ferromagnetic) phase, so that the random quantum critical point is at $\delta = 0$.

In the Ma-Dasgupta-Hu RG-method the strongest term in the Hamiltonian, coupling or field, of strength Ω are successively decimated out and the neighboring fields or couplings are replaced by weaker ones, which are generated by a perturbation calculation. The basic RG-equations for coupling and field decimations are given by:

$$\tilde{h} = \frac{h_i h_{i+1}}{J_i \kappa} \quad , \quad \tilde{J} = \frac{J_{i-1} J_i}{h_i \kappa} \quad , \quad (3)$$

respectively, which are related through duality. Here, for the RTIM $\kappa = 1$. Under renormalization we follow the probability distributions of the couplings, $R(J, \Omega)$, and that of the fields, $P(h, \Omega)$. When the energy-scale is lowered as $\Omega \rightarrow \Omega - d\Omega$ the distribution of the couplings is changed as:

$$\frac{dR(J, \Omega)}{d\Omega} = R(J, \Omega)[P(\Omega, \Omega) - R(\Omega, \Omega)] - P(\Omega, \Omega) \int_{J\kappa}^{\Omega} dJ' R(J', \Omega) R\left(\frac{J\Omega\kappa}{J'}, \Omega\right) \frac{\Omega\kappa}{J'} \quad , \quad (4)$$

where the first term in the r.h.s. is due to a balance between decimated couplings and normalization, whereas the second term accounts for the generated new couplings. A similar equation for the field distribution follows from Eq.(4) through duality

$$\frac{dP(h, \Omega)}{d\Omega} = P(h, \Omega)[R(\Omega, \Omega) - P(\Omega, \Omega)] - R(\Omega, \Omega) \int_{h\kappa}^{\Omega} dh' P(h', \Omega) P\left(\frac{h\Omega\kappa}{h'}, \Omega\right) \frac{\Omega\kappa}{h'} \quad , \quad (5)$$

which amounts to interchange $J \leftrightarrow h$ and $R \leftrightarrow P$.

For the RTIM, i.e. for $\kappa = 1$, we found one class of solutions of the RG equations in the form:

$$R(J, \Omega) = R(\Omega, \Omega) (\Omega/J)^{1-R(\Omega, \Omega)\Omega} \\ P(h, \Omega) = P(\Omega, \Omega) (\Omega/h)^{1-P(\Omega, \Omega)\Omega} \quad , \quad (6)$$

where the distributions involve the parameters, $\tilde{R}(\Omega) \equiv R(\Omega, \Omega)$ and $\tilde{P}(\Omega) \equiv P(\Omega, \Omega)$, which satisfy the relation $(\tilde{P} - \tilde{R})\Omega = 1/z = \text{const}$. Thus the solution is characterized by one parameter, $z = z(\delta)$, which depends on the quantum control-parameter, δ : at the critical point, $1/z(0) = 0$, whereas in the paramagnetic phase, $\delta > 0$, $1/z(\delta) > 0$ and monotonically increases with δ .

In terms of the variables, $y = \tilde{R}\Omega + 1/2z = \tilde{P}\Omega - 1/2z$ and $x = -\ln \Omega$ we obtain the differential equation:

$$\frac{dy}{dx} + y^2 = \frac{1}{4z^2} \quad , \quad (7)$$

which has the solution, $y = 1/(x - x_0)$, $x_0 = \text{const}$, at the critical point with $1/z = 0$. The distribution of $\rho = R\Omega$ in terms of the variable $\eta = -(\ln \Omega - \ln J)/\ln \Omega$ is given

by $\rho(\eta)d\eta = \exp(-\eta)d\eta$, which corresponds to the fixed-point solution by Fisher [8]. At this point we refer to Fisher's analysis [8] and conclude that the functions in Eqs(6) indeed represent the fixed-point distribution for all non-singular initial distributions.

In the Griffiths phase, $\delta > 0$, the solution of Eq.(7) in terms of the original energy-scale variable, Ω , is given by

$$y = \frac{y_0/2z + 1/4z^2 \tanh[\ln(\Omega_0/\Omega)/2z]}{1/2z + y_0 \tanh[\ln(\Omega_0/\Omega)/2z]} \quad , \quad (8)$$

where $y = y_0$ at a reference point, $\Omega = \Omega_0$. Approaching the line of semi-critical fixed points, i.e. for $\Omega/\Omega_0 \rightarrow 0$, we have to leading order:

$$\tilde{R}\Omega = \tilde{P}\Omega - 1/z = \tilde{R}(\Omega_0)/[\tilde{P}(\Omega_0)z] (\Omega/\Omega_0)^{1/z} + \dots \quad (9)$$

thus \tilde{P} and \tilde{R} have different low energy asymptotics.

The *physical relevance* of $1/z$ can be obtained by studying the change of number of spins, $n_\Omega \rightarrow n_\Omega - dn_\Omega$ connected with a change in the energy scale as $\Omega \rightarrow \Omega - d\Omega$. This leads to the differential equation $dn_\Omega/d\Omega = n_\Omega [P(\Omega, \Omega) + R(\Omega, \Omega)]$, the solution of which is given by:

$$n_\Omega = \{\cosh[\ln(\Omega_0/\Omega)/2z] + 2z y_0 \sinh[\ln(\Omega_0/\Omega)/2z]\}^{-2} \quad , \quad (10)$$

which along the line of semi-critical fixed points has the asymptotic behavior $n_\Omega = \text{const } \Omega^{1/z}$, $\Omega \rightarrow 0$. Since the typical distance between remaining spins is $L_\Omega \sim 1/n_\Omega \sim \Omega^{-1/z}$, we can identify z as the *dynamical exponent*, which governs the relation between time- and length-scales as $\tau \sim L^z$.

Next we show that z is invariant along the RG trajectory and can be deduced from the original distributions. For this we consider the averages, $[J^\mu]_{\text{av}}$ and $[h^{-\mu}]_{\text{av}}$, and using Eqs.(4) and (5) we calculate the derivative:

$$\cdot \frac{d}{d\Omega} [(J/h)^\mu]_{\text{av}} = (1 - [(J/h)^\mu]_{\text{av}}) \\ \times (P(\Omega, \Omega)\Omega^{-\mu} [J^\mu]_{\text{av}} + R(\Omega, \Omega)\Omega^\mu [h^{-\mu}]_{\text{av}}) \quad (11)$$

which is vanishing for $\mu = \tilde{\mu}$, if $[(J/h)^{\tilde{\mu}}]_{\text{av}} = 1$. Consequently $\tilde{\mu}$ stays invariant along the RG trajectory until the fixed point, where using the distribution in Eqs.(6) we obtain $\tilde{\mu} = 1/z$. Thus the dynamical exponent for the RTIM is given by the solution of the equation:

$$\left[(J/h)^{1/z}\right]_{\text{av}} = 1 \quad , \quad (12)$$

which is then exact, since the RG-transformation becomes asymptotically exact as $\Omega \rightarrow 0$. This latter statement follows from the fact that the ratio of decimated bonds, Δn_J , and decimated fields, Δn_h , goes to zero as $\Delta n_J/\Delta n_h = R(\Omega, \Omega)/P(\Omega, \Omega) \sim \Omega^{1/z}$. Then the probability, $Pr(\alpha)$, that the value of a coupling, J , being neighbor to a decimated field is $\Omega < J < \alpha\Omega$ with $0 < \alpha < 1$ is given by $Pr(\alpha) = 1 - \alpha^{\tilde{R}\Omega}$, which goes to zero for any

non-zero α , since $\tilde{R}\Omega \sim \Omega^{1/z}$ at the fixed point. Consequently the decimations in Eq.(3) and the related RG equation in Eqs.(4) and (5) are indeed exact.

The relation in Eq.(12) can be recovered starting from the exact expression for the surface magnetization, m_s , on a chain with a fixed spin at site $L+1$ [14,10]:

$$\frac{1}{m_s^2} = 1 + \sum_{l=1}^L \prod_{i=1}^l \left(\frac{h_i}{J_i} \right)^2. \quad (13)$$

This type of expression is the so-called Kesten-variable in the mathematical literature [15] and the corresponding probability distribution is singular at $m_s = 0$ in the thermodynamic limit for $[\ln J]_{\text{av}} > [\ln h]_{\text{av}}$ [15,16]. Then for the distribution of $\ln m_s$ we have the following singularity:

$$P(\ln m_s) \sim m_s^{1/\tilde{z}}, \quad m_s \rightarrow 0, \quad (14)$$

where \tilde{z} is the solution of Eq.(12) in terms of the dual variables. The physical origine of the small m_s tail of the distribution is due to such samples which have a weakly coupled domain (WCD), which effectively cuts the system into two very weakly interacting parts and thus reduces the surface order enormously. In the dual system in the paramagnetic phase the dual object to a WCD is a strongly coupled domain (SCD) which results in a very small energy gap, ϵ . Thus in the tails of the distributions, m_s and ϵ are dual quantities. This remark indicates that the dynamical exponent found by the RG calculation in Eq.(12) is indeed exact [17].

Next, we consider general random quantum spin chains with a critical IRFP and analyze the structure of the RG equations close to the line of semi-critical fixed points, thus as $\Omega \rightarrow 0$. As for the RTIM, the decimation for fields and couplings is asymmetric and for $\Omega \rightarrow 0$ exclusively fields are decimated out, which are typically infinitely stronger, than the neighboring couplings. Therefore the RG decimation equations in Eq.(3) are asymptotically exact. The second point is to show that the dynamical exponent stays invariant along the RG trajectory, even though in the starting phase the RG equations are approximative. For this we consider the low energy tail of the distribution function of the first gap, $P_1(\ln \epsilon)$, which involves in analogy to Eq.(14) the exponent z , and use the scaling result of Ref [18]. This states that the probability distribution of the second, third, etc. gaps are related to $P_1(\ln \epsilon)$ as $P_2(\ln \epsilon) \sim P_1^2(\ln \epsilon)$, $P_3(\ln \epsilon) \sim P_1^3(\ln \epsilon)$, etc, due to the fact that for a small second, third gap one needs two, three independent SCD-s and the corresponding probabilities are multiplied. In the RG decimation the SCD-s are only eliminated through coupling decimation, since their couplings are stronger than the average fields. If at some time a SCD with a small gap, ϵ , is eliminated then in the probability distribution, $P_1(\ln \epsilon)$, one should consider the former second

gap and use the corresponding conditional probability, $P_1(\ln \epsilon) \rightarrow P_2(\ln \epsilon)/P_1(\ln \epsilon) \sim P_1(\ln \epsilon)$. Thus the small energy tail of the gap-distribution and consequently the dynamical exponent remains invariant under the renormalization procedure. The previously obtained exact results for the RTIM give strong support for the validity of these phenomenological considerations.

For a numerical demonstration of the validity of the above statement we considered two random quantum spin chains, the dimerized Heisenberg (XXX) chain and the q -state RQPM, both having a set of RG equations very similar to that of the RTIM in Eq.(3). For the dimerized XXX chain J and h in Eq.(3) are replaced by the Heisenberg couplings at odd and even positions, J_o and J_e , respectively, and the parameter takes the value $\kappa = 2$ [6,9]. The distance from the critical point is measured similarly to Eq.(2). For the q -state RQPM fields and couplings play analogous rôle as for the RTIM, the quantum control-parameter is given in Eq.(2), whereas κ takes the value $\kappa = q/2$ [19]. We note that the RG equations for the XXX-chain and the $q = 4$ state RQPM are identical.

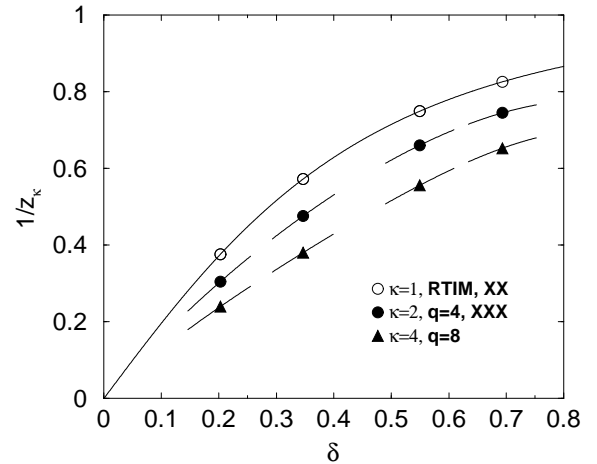


FIG. 1. Dynamical exponents from numerical iteration of the RG-equations in Eq.(3) for different values of the parameter κ . For $\kappa = 1$, which corresponds to the RTIM and the random dimerized XX-chain the exact result is given by the full line, for $\kappa = 2$ and 4 the broken lines are guide to the eye.

At the critical point the RG-equations for $1 \leq \kappa < \infty$ has been solved by Senthil and Majumdar [19] with the result that κ is an irrelevant variable and the IRFP is the same as for the RTIM. In the Griffiths-phase we could not find a complete solution of the RG equations, in spite of the close similarity to that of the RTIM. We could, however, show that up to an accuracy of $O(\Omega^{1/z})$ the solution is of the form of Eqs.(6) and thus there is infinite randomness along the line of fixed points. The z exponent, however, does depend on the parameter κ , since the validity of the condition in Eq.(12) is limited to $\kappa = 1$, thus

in general $z = z_\kappa(\delta)$.

We have calculated the dynamical exponent by a numerical implementation of the RG scheme over 50000 samples of length $L \leq 2^{14}$. Starting with the uniform probability distribution: $R_0(J) = \Theta(1 - J)\Theta(J)$, $P_0(h) = \Theta(h_0 - h)\Theta(h)/h_0$ (and analogously for the XXX-chain) we got the estimates shown in Fig.1: $1/z_\kappa$ is a monotonously decreasing function of κ and eventually it goes to zero in the whole Griffiths phase in the limit $\kappa \rightarrow \infty$.

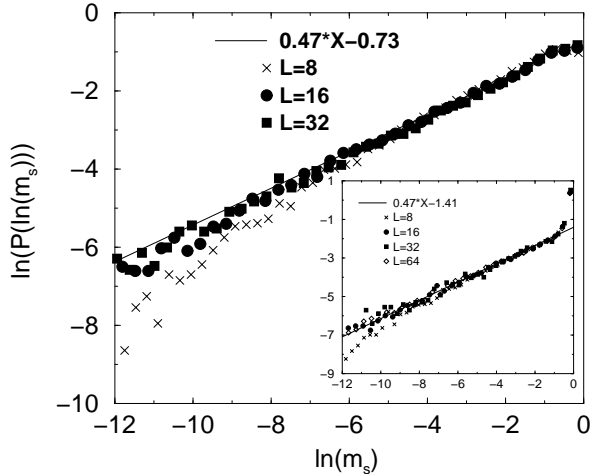


FIG. 2. Probability distribution of the logarithm of the surface magnetization of the dimerized random XXX-chain with $\delta = -(\ln 2)/2$ for different finite systems calculated by the DMRG method. The full straight line with a slope $1/z(\delta) = .47$ represents the asymptotic behavior according to the RG method, as given in Fig. 1. In the inset the same quantity is shown for the $q = 4$ state RQPM at the same distance from the critical point. The asymptotic slope of this distribution can be well fitted by the same exponent as for the XXX-model.

The dynamical exponents of the XXX-chain and the RQPM are also calculated directly from the asymptotic behavior of the distribution of the surface magnetization, as given in Eq.(14). For the numerical calculations of the surface magnetizations we used the DMRG method for rather large finite chains with $L \leq 64$ and considered some 20000 samples. We found an overall agreement between the dynamical exponents calculated by the two methods. As a demonstration we show in Fig. 2 the distribution of m_s for the XXX-chain, compared with that of the $q = 4$ state RQPM, where for both models we are at the same distance from the transition point. As seen in Fig. 2 the asymptotic behavior of the two distributions is identical, as expected on the RG basis, since $\kappa = 2$ for both models. Furthermore the dynamical exponents agree very well with those calculated by the RG method.

To conclude, we have shown in this paper that for ran-

dom quantum spin chains the RG method of Ma, Dasgupta and Hu is asymptotically exact for large times, i.e. along the line of semi-critical fixed points. Consequently the dynamical exponent in the Griffiths phase calculated by the RG-method is exact. This result will hopefully stimulate new efforts to solve the RG equations for different systems analytically in 1d also outside the critical point, and in higher dimensions to perform numerical calculations and get more precise estimates for the Griffiths-McCoy singularities.

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